

# IQI 04, Seminar 13

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- Quantum physics simulation.

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## Quantum Physics Simulation

- Superficial problem statement.  
Given: A model of a quantum physics system.  
Problem: Determine a physical quantity.
  - A model of quantum physics may be characterized by
    1. a Hamiltonian  $H$  generating unitary evolution in
    2. a state space  $\mathcal{H}$  of wavefunctions.
  - Some physical quantities. [Complexity for "physical"  $H, A, B, \dots$ ]
    - The lowest energy of  $H$ . [In general: Hard]
    - The spectrum of  $H$ . [Complete: Hard. With resolution  $\epsilon$ : Q. easy.]
    - The partition function  $Z(\beta) = \text{tr}(e^{-\beta H})$ . [Quadratic q. speedup]
    - Thermodyn. expectations  $\text{tr}(e^{-\beta H} A) / Z(\beta)$ . [Quad. q. speedup]
    - Expectations  $\langle \psi | A | \psi \rangle$  for known states  $|\psi\rangle$ . [Q. easy to within  $\epsilon$ ]
    - Correlation functions  $\langle \psi | e^{iHt} A e^{-iHt} B | \psi \rangle$ . [Q. easy to within  $\epsilon$ ]
    - Response to probes under experimental conditions.
- ["virtual" experiment is q. easy]



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  2. a state space  $\mathcal{H}$  of wavefunctions.
- Example models.
  - A particle of mass  $m$  in one dimension.  
 $\mathcal{H}$ : Square integrable functions on  $\mathbb{R} = (-\infty, \infty)$ .  
 $H = -\frac{1}{m} \frac{\partial^2}{\partial x^2} + V$ . [...  $\hbar = 1$ ]  
Unitary evolution according to Schrödinger's equation:  $\frac{\partial}{\partial t} \psi = -iH\psi$ .
  - $N$  particles in 3 dimensions.  
 $\mathcal{H}$ : Square integrable functions on  $\mathbb{R}^{3N}$ .  
 $H = \sum_{j=1}^N E_j(\text{kinetic}) + V_j(\text{potential}) + \sum_{1 \leq j < k \leq N} I_{j,k}(\text{interaction})$
  - Translation invariant 1-D lattice of spin- $\frac{1}{2}$  systems.  
 $H = \sum_k H_I^{(k,k+1)}$ , with  $H_I^{(k,k+1)} = \sum_{u,v} \alpha_{u,v} \sigma_u^{(k)} \sigma_v^{(k+1)}$



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## Physics Simulation Algorithms: Common Features

- Discretization and finitization of the model.
    - Particle of mass  $m$  in one dimension.
- Wavefunction:  $\psi(x), x \in \mathbb{R}$ .  
 $x \in \{-B, \dots, 0, B\frac{1}{N}, \dots, B\}$ .

Hamiltonian:  $-\frac{1}{m} \frac{\partial^2}{\partial x^2} + V(x)$        $\sum_x \frac{1}{m} F x^2 |x\rangle \langle x| F^\dagger + V(x) |x\rangle \langle x|$   
 ...  $F$  is the Fourier transform.
- Faithful realization in a finite number of qubits.
    - $|-B + r/N\rangle \rightarrow |r\rangle$ ,  $r$  in binary.
  - Implementation of evolution.
    - $\mathbf{K} = F \sum_x \frac{1}{m} x^2 |x\rangle \langle x| F^\dagger$ ,  $\mathbf{V} = \sum_x V(x) |x\rangle \langle x|$ .  
 Trotterization:  $e^{-iHt} = (e^{-i\mathbf{K}t/T} e^{-i\mathbf{V}t/T})^T + O(1/T)$
  - Information extraction: State preparation and measurement.

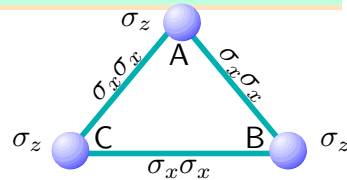


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## Faithful Evolution

- Example: Triangle  $XY$ -model.

- Three spin- $\frac{1}{2}$  systems A, B, C.
- Hamiltonian:

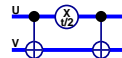


$$H = \sigma_z^{(A)} + \sigma_z^{(B)} + \sigma_z^{(C)} + \sigma_x^{(A)} \sigma_x^{(B)} + \sigma_x^{(A)} \sigma_x^{(C)} + \sigma_x^{(B)} \sigma_x^{(C)}$$

Each term in  $H$  is readily simulatable.

$$e^{-i\sigma_z^{(U)} t} : \quad \text{A } z\text{-rotation.} \quad \text{U} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$e^{-i\sigma_x^{(U)} \sigma_x^{(V)} t} : \quad \text{Conjugate of an } x\text{-rotation by cnots.}$$



But the terms do not all commute. Combine commuting terms:  
 $H_{int} = \sigma_z^{(A)} + \sigma_z^{(B)} + \sigma_z^{(C)}, H_{cpl} = \sigma_x^{(A)} \sigma_x^{(B)} + \sigma_x^{(A)} \sigma_x^{(C)} + \sigma_x^{(B)} \sigma_x^{(C)}.$   
 $e^{-iH_{int}t} = e^{-i\sigma_z^{(A)}t} e^{-i\sigma_z^{(B)}t} e^{-i\sigma_z^{(C)}t}, \text{ similarly for } e^{-iH_{cpl}t}.$

Trotterize: 
$$e^{-iHt} = \left( e^{-iH_{int}\frac{t}{N}} e^{-iH_{cpl}\frac{t}{N}} \right)^N + O(|H|^2 \frac{t^2}{N})$$

$$e^{-iHt} = \left( e^{-iH_{int}\frac{t}{2N}} e^{-iH_{cpl}\frac{t}{N}} e^{-iH_{int}\frac{t}{2N}} \right)^N + O(|H|^3 \frac{t^3}{N^2})$$

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## The Virtual Quantum Physics Lab

- Quantum computers can efficiently simulate an experimental procedure on a specified quantum system.
- Requirements:
  - ✓ Qubit representation of the quantum system.
  - ✓ Evolution of its internal Hamiltonian.
  - ✓ Simulation of coupling to experimental probes.
- Preparation of a physically meaningful initial state.
- Implementation of measurements with noise no worse than the actual experiment would have.

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## Simulatability of Physical Systems

### Physical universality thesis for quantum computers.

Given: Physical system  $S$ .

Physical Hamiltonian  $H \geq 0$  for  $S$ .

Physically meaningful state  $|\psi\rangle$  of  $S$  of av. energy  $E$ .

Then: It is possible to represent  $S$ ,  $H$  and  $|\psi\rangle$  on qubits, and evolve  $H$  for time  $t$  using quantum gates, with resources polynomial in

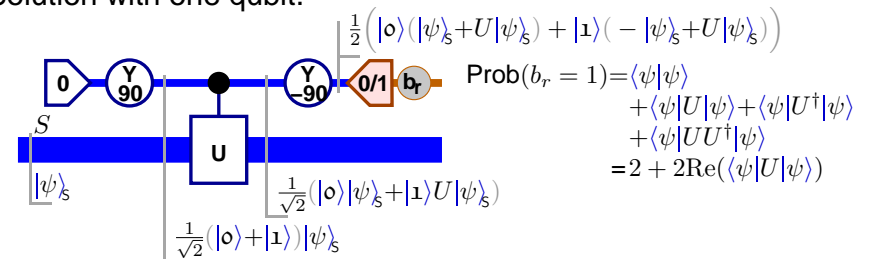
$E$ ,  $t$  and the approximation error.

- Evidence: No counterexample so far. . . .
- Typical representation relationships:
  - $S$  can be approximated by  $N$  degrees of freedom.
  - Hamiltonian: Sum of pairwise interactions between degrees of freedom.
  - The energy is linear (maybe quadratic) in  $N$ .
  - A degree of freedom can be approximated by a “small” qubit register.
  - Simulating an arbitrary interaction on a pair of small registers is “efficient”.

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## Measuring Unitary Expectations

- Given: Quantum system  $S$ , preparable in state  $|\psi\rangle$ .  
 Unitary  $U^{(S)}$ , with “controlled” implementations.  
 Problem: Measure  $\langle\psi|U|\psi\rangle$  to within  $\epsilon$ .
- Solution with one qubit.



- Get  $\text{Re}\langle\psi|U|\psi\rangle$  from  $\text{Prob}(b_r = 1) \pm \epsilon/2$ .
- To obtain  $\text{Im}\langle\psi|U|\psi\rangle$ , replace  $U$  by  $iU$ .
- Requires  $O(1/\epsilon^2)$  repetitions.

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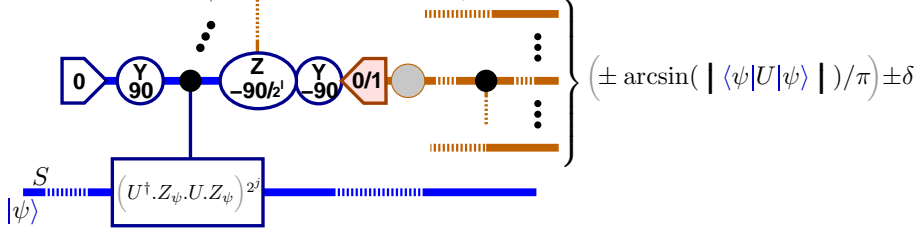
## Measuring Unitary Expectations

- Given: Quantum system  $S$ , preparable in state  $|\psi\rangle$ .  
Unitary  $U^{(S)}$ , with “controlled” implementations.

Problem: Measure  $\langle\psi|U|\psi\rangle$  to within  $\epsilon$ .

- Solution with amplitude estimation.

Assume that  $Z_\psi = \text{“selective } -1 \text{ of } |\psi\rangle\text{”}$  is implementable.



- Obtain  $|\langle\psi|U|\psi\rangle|$  from  $\pm \arcsin(|\langle\psi|U|\psi\rangle|/\pi) \pm \delta$ .
- Infer  $\langle\psi|U|\psi\rangle$  by doing the same with  $U' = U^{(S)}|0\rangle_A\langle 0| \pm |1\rangle_A\langle 1|$  and  $|\psi'\rangle = |\psi\rangle_S + |0\rangle_A$ .
- Requires  $O(1/\epsilon)$  coherent, controlled applications of  $U$ .

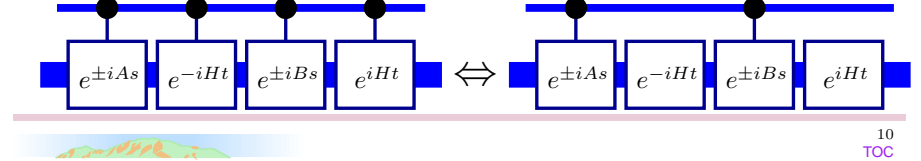
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## Measuring Correlation Functions

- Given: Quantum system  $S$ , preparable in state  $|\psi\rangle$ .  
Operators  $A$  and  $B$ , implementable as needed.

Problem: Measure  $\langle\psi|e^{iHt}Be^{-iHt}A|\psi\rangle$  to within  $\epsilon$ .

- If  $A$  and  $B$  are unitary, let  $U = e^{iHt}Be^{-iHt}A$  and measure  $\langle\psi|U|\psi\rangle$  to within  $\epsilon$ .
- $A$  and  $B$  are Hermitian. Let  $B(t) = e^{iHt}Be^{-iHt}$ 
  - Obtain  $S = \sum_{a,b=0,1} (-1)^{a+b} \langle\psi|e^{(-1)^a iB(t)} e^{(-1)^b iAs}|\psi\rangle \pm \delta$ .
  - $S = 4(s^2 \langle\psi|B(t)A|\psi\rangle + O((|A| + |B|)^3 s^3)) \pm \delta$ .
  - Set  $t = O(\epsilon/(|A| + |B|)^3)$ ,  $\delta = O(\epsilon s^2)$ .
- Requires  $O((|A| + |B|)^3/\epsilon^3)$  uses of  $e^{(-1)^a iB(t)} e^{(-1)^b iAs}$ .
- Note network simplification:



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## Measuring Hermitian Expectations

- Given: Quantum system  $S$ , preparable in state  $|\psi\rangle$ .  
Hermitian  $A^{(S)}$  with  $e^{-itA}$  implementable.

Problem: Measure  $\langle\psi|A|\psi\rangle$  to within  $\epsilon$ .

- Solution using unitary expectation measurements.

- For small  $t$ ,  $e^{-iAt} = 1 - itA + O(|A|^2 t^2)$ .  
 $\langle\psi|e^{-iAt}|\psi\rangle = 1 - it\langle\psi|A|\psi\rangle + O(|A|^2 t^2)$
  - Choose  $t$  such that  $O(|A|^2 t^2)$  contributes at most  $t\epsilon/2$ .  
 $t = O(\epsilon/|A|^2)$
  - Measure  $\langle\psi|e^{-iAt}|\psi\rangle$  to within  $t\epsilon/2$ .
- Requires  $O(|A|^2/\epsilon^2)$  uses of  $e^{-iAt}$  with amp. estimation.

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## Measuring Spectra

- Given: Quantum system  $S$  with Hamiltonian  $H$ .

Problem: Measure the spectrum of  $H$ .

Spectrum of  $H$ : Multiset  $\{\lambda_k\}_k$  of eigenvalues of  $H$ .

- Measuring the full spectrum is typically exponentially hard.
- Spectral density with resolution  $\epsilon$  and signal-to-noise (SNR)  $S$ .
  - Measure  $f(t) = \text{tr}(e^{-iHt})/N \pm \delta$  for  $t = 0, \dots, (M-2)\Delta, (M-1)\Delta$ .

Note:  $\text{tr}(e^{-iHt})/N = \langle\psi|e^{-iHt}|\psi\rangle$  for  $|\psi\rangle = \frac{1}{\sqrt{N}} \sum_k |k\rangle_S |k\rangle_{S'}$ .

- Compute the discrete Fourier transform  $\hat{f}$  of  $f$ .

$$\begin{aligned} f(l\Delta) &= \sum_k e^{-i\lambda_k \Delta l} / N \\ \hat{f} &= \frac{1}{\sqrt{M}} \sum_l f(l\Delta) e^{i2\pi l/M} \end{aligned}$$

Range:  $\frac{1}{\Delta} > |H|$ . Resolution:  $\frac{1}{M\Delta} < \epsilon$ . SNR:  $\delta < 1/S$ .

- Requires  $O(|H|S/\epsilon)$  uses of  $e^{-iHt}$  with  $t$  up to  $O(1/\epsilon)$ .

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## State preparation Problems

- Prepare the ground state of  $H$ ?  
... appears to be difficult in general.
- Prepare a thermodynamic state  
with density matrix  $e^{-\beta H} / \text{tr}(e^{-\beta H})$ ?  
... can simulate contact with a thermal bath, but efficiency?

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